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Interactive comment on "A fast stratospheric chemistry solver: the E4CHEM submodel for the atmospheric chemistry global circulation model EMAC" *by* A. J. G. Baumgaertner et al.

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The authors are grateful for the valuable comments by the referee. The referee's only major reservation is the missing representation of bromine chemistry, similar to the comment by referee #1. As indicated in the manuscript, an extension of the chemical algorithm is currently under development and will be published separately. For the meantime, we have optionally included the parameterisation of ozone depletion by bromine developed by Rex et al. (2003) and implemented for CHEM by Stenke et al. (2009). The motivation for this manuscript was merely to document (and evaluate the performance) of the modifications of CHEM (available for ECHAM4) for the new

ECHAM5 based EMAC system, or in other words to show that during the transition the algorithms are not deteriorated and that the results of the new system are in sufficient agreement with the alternative, more complex (but more flexible) approach of MECCA. We completely agree that scientific production simulations should not be performed without Br-Chemistry. However, additional evaluations of E4CHEM extensions are beyond the scope of this manuscript. We will include these arguments this in the revised manuscript.

Replies to specific comments:

"Why not say what the difference in the computational cost are...": We will list the computational costs of the performed simulations (boxmodel and 3-D) in the revised manuscript. Note however that this very much depends on the configuration and setup of the simulations. For example, the applied type of scavenging is computationally much more efficient than the type used in other studies with EMAC. "The CPU time consumed by the CAABA simulations with E4CHEM or MECCA switched on was measured on an IBM Power6 architecture using simulation lengths of 30 days. The E4CHEM simulations need approximately 5 – 35% less CPU time than the MECCA simulation with the equivalent chemistry setup, depending on the compiler optimization level. Note that a significant part of the performance increase in the chemistry is concealed by the JVAL submodel as well as other parts of CAABA (e.g. output routines) which also require a significant amount of CPU time. If all other subroutines are switched off, the E4CHEM simulation requires 80% less CPU time than the MECCA simulation." and for 3D: "We measured the consumed CPU time for the simulations presented above, which were performed on an IBM POWER6 computer using 16 nodes with 64 threads each. The average CPU time consumed by each model time step was 0.47 s for S-MECCA(E4CHEM), 0.17 s for S-E4CHEM (a performance increase of 64% compared to the S-MECCA(E4CHEM) simulation), and 1.3 s for S-MECCA(EVAL) (275% slower than the S-MECCA(E4CHEM) simulation)."

"Isn't the point to have the same reaction rates?!": For the box model, we performed

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simulations using the original and updated reaction rates. The concerned sentence in the abstract refers to the original rates. We will rewrite this to make this clearer: “With the original reaction rates, for some species the steady state in the box model differs by up to 100% when compared to results from CAABA/MECCA, but after an update of the reaction rates satisfactory agreement was reached.”

We will add the reference to the CCMVal report as requested.

Sedimentation of NAT: This issue is discussed in more detail in the paper by Steil et al. (2003). In the model it is assumed that ice forms on large NAT particles, when the icepoint is reached (Carslaw et al., 1997). Therefore the sedimentation velocity of NAT and ice is assumed to be identical if ice is present, otherwise sedimentation is neglected, assuming that most NAT-particles are too small to sediment significantly. This scheme may underestimate denitrification in the Arctic but is well suitable for the Antarctic lower stratosphere where ice particles occur frequently. So-called “NAT-rocks” (e.g. Fahey et al., 2001), which have sizes large enough to sediment without any ice present, are not captured. This also may contribute to an underestimation of denitrification in the Arctic. Nevertheless, we agree that the PSC-scheme might need an update to be more competitive with the schemes used in EMAC, but this isn’t likely to affect the computational performance of E4CHEM.

Supercooled ternary solution representation for sulfate based PSC: The study presented here did not include type Ib (STS) sulfate-based PSCs since we documented here the status of the code as presented in Steil et al. (2003). Later, undocumented versions of CHEM included an extension where this was applied. We will mention this in the revised manuscript.

Page 188 Lines 6-9: We will remove the selection string from the updated manuscript. We have excluded bromine chemistry from EMAC/MECCA because CHEM, and therefore EMAC/E4CHEM, does not contain bromine chemistry, see the discussion above.

References:

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Interactive comment on Geosci. Model Dev. Discuss., 3, 181, 2010.